

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $7.35 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $7.93 \times 10^{-1}$

**Confidence level:**  $7.77 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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1-Propanol

**Measured:**  $5.53 \times 10^{-12}$

**Predicted:**  $7.35 \times 10^{-12}$

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Isopropanol

**Measured:**  $5.07 \times 10^{-12}$

**Predicted:**  $5.72 \times 10^{-12}$

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1,4-Diazabicyclo[2.2.2]octane

**Measured:**  $2.20 \times 10^{-11}$

**Predicted:**  $1.30 \times 10^{-11}$

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1-Butanol

**Measured:**  $8.57 \times 10^{-12}$

**Predicted:**  $1.06 \times 10^{-11}$

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2-Butanol

**Measured:**  $9.60 \times 10^{-12}$

**Predicted:**  $8.64 \times 10^{-12}$